LA-UR-93-4019 submitted to *Molec. Phys.* 2/5/2008

Comparison of Electron Density Functional Models

Gary G. Hoffman † *and Lawrence R. Pratt* *

Abstract

Presented here are calculations of the distortion of the density of an electron gas due to the electrostatic field of a proton. Several models based upon the local density approximation (LDA) of density functional theory [linear response theory, Kohn-Sham (KS), optimized Thomas-Fermi theory (OTF), and OTF plus perturbation corrections] are compared with one another. These models, in turn, are compared with available results of quantum Monte Carlo (QMC) calculations for the same system. Comparison of the KS results with the OTF results shows a very reasonable agreement that seems to be progressively improvable. This provides encouragement for the application of the OTF model to condensed phase systems. The QMC calculations of the density do not agree well with the density functional results. The reasons for this poor agreement are not clear. This particular system is expected to be an ideal one for application of the LDA and, thus, the poor agreement is of fundamental importance. The lack of detail presented in the available QMC results leads us to conclude that the QMC calculations should be attempted again.

† *Department of Chemistry, Florida International University, Miami, FL 33199*

* *Los Alamos National Laboratory, Los Alamos, NM 87545.*

published as: *Molec. Phys.* **82**, 245-261(1994)